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# Diffuse scattering from dodecagonal quasicrystals

Jianlin Lei[1,2,a], Renhui Wang[1,2], Chengzheng Hu[1], and Di-hua Ding[1]

[1] Department of Physics, Wuhan University, Wuhan 430072, P.R. China
[2] Beijing Laboratory of Electron Microscopy, Institute of Physics and Center for Condensed Matter Physics, Chinese Academy of Sciences, P.O. Box 2724, Beijing 100080, P.R. China

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**Abstract.** General formulae for thermal diffuse scattering from quasicrystals are applied to the case of dodecagonal quasicrystals from corresponding elasticity theory. Contours of constant diffuse scattering intensity are illustrated. Unlike ordinary crystals, shapes of isointensity contours are much more complicated and vary even among the collinear Bragg spots. Diffuse scattering patterns in the plane perpendicular to a given zone axis are associated with corresponding specific elastic constants. Information about elastic constants can be extracted from quantitative analysis of diffuse scattering patterns.

**PACS.** 61.44.Br Quasicrystals

## 1 Introduction

Since the discovery of the quasicrystalline icosahedral phase in rapidly quenched Al-Mn alloy [1], much effort has been paid to the studies of such new materials. The striking characteristic of quasicrystals is the existence of sharp Bragg peaks. However, distortion and peak broadening observed in diffraction patterns revealed some systematic deviations from the ideal quasicrystal model [2,3]. Strains in phonon and phason variables or quenched dislocations have been invoked to account for experimental observation of peak positions and peak widths in some detail [4,5]. Socolar and Wright have examined the distinctive shapes of Bragg spots observed in icosahedral phases and constructed a uniform phason strain field within a grain that reproduced the experimental peak shapes [6]. Jaric and Nelson [7] have developed an alternative theory of diffuse scattering from incommensurate crystals and quasicrystals due to spatially fluctuating thermal and quenched strains and applied their derived general formulae to a specific case of icosahedral quasicrystals according to elastic properties of icosahedral quasicrystals which have been examined intensively [8–11]. With the help of this theory, the onset of hydrodynamic instability of icosahedral phases has been discussed [12,13]; the diffuse scattering located close to Bragg reflections has been studied as a function of the temperature on a single grain of the Al-Pd-Mn icosahedral phase using elastic neutron scattering and the ratio of two phason elastic constants was obtained [14,15]. Recently, we discussed diffuse scattering from decagonal [16], octagonal [17] and pentagonal quasicrystals [18].

Dodecagonal quasicrystals were observed experimentally in $Cr_{70.6}Ni_{29.4}$ [19], $Ni_2V_3$, $Ni_{10}SiV_{15}$ [20] and Ta-Te [21] alloys. Elasticity of planar quasicrystals with twelvefold symmetry was discussed in some papers [22–24]. Recently, significant progress has been made in studying the elastic properties of two-dimensional (2D) quasicrystals including dodecagonal quasicrystals by some authors [25–27]. Based on the 5D crystallographic symmetry operations listed by Janssen [28], they have derived all possible point groups of 2D quasicrystals of rank 5 and calculated the numbers of independent forth-rank elastic constants of 2D quasicrystals with group representation theory. Here and hereafter, a 2D quasicrystal refers not to a real plane but to a 3D solid with 2D quasiperiodic and 1D periodic structure.

In this paper, we will restrict our attention to dodecagonal quasicrystals. Diffuse scattering from dodecagonal quasicrystals is formulated in Section 3 according to elastic properties of dodecagonal quasicrystals summarized in Section 2. Isointensity contours of diffuse scattering are calculated using the derived formulae and analysis of the results are given in Section 4. The coordinate systems which we use for dodecagonal quasicrystals are given in Appendix.

## 2 Point groups, Laue classes and elastic properties of dodecagonal system

In this section we will illustrate the determination of explicit forms of invariant terms in the elastic energy and elastic constant tensor for dodecagonal system. We would like to limit the brief description of this method to a minimum necessary for the calculation. A more detailed discussion can be found in the literature [24–27].

If an analytic expression of the elastic free energy is possible, it will be quadratic in the spatial gradients of

[a] e-mail: jlei@usa.net

**Table 1.** Character table for the point group $C_{12v}$.

| | $\varepsilon$ | $\alpha$ | $\alpha^2$ | $\alpha^3$ | $\alpha^4$ | $\alpha^5$ | $\alpha^6$ | $\beta$ | $\alpha\beta$ |
|---|---|---|---|---|---|---|---|---|---|
| $\Gamma_1$ | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| $\Gamma_2$ | 1 | 1 | 1 | 1 | 1 | 1 | 1 | −1 | −1 |
| $\Gamma_3$ | 1 | −1 | 1 | −1 | 1 | −1 | 1 | 1 | −1 |
| $\Gamma_4$ | 1 | −1 | 1 | −1 | 1 | −1 | 1 | −1 | 1 |
| $\Gamma_5$ | 2 | $\sqrt{3}$ | 1 | 0 | −1 | $-\sqrt{3}$ | −2 | 0 | 0 |
| $\Gamma_6$ | 2 | 1 | −1 | −2 | −1 | 1 | 2 | 0 | 0 |
| $\Gamma_7$ | 2 | 0 | −2 | 0 | 2 | 0 | −2 | 0 | 0 |
| $\Gamma_8$ | 2 | −1 | −1 | 2 | −1 | −1 | 2 | 0 | 0 |
| $\Gamma_9$ | 2 | $-\sqrt{3}$ | 1 | 0 | −1 | $\sqrt{3}$ | −2 | 0 | 0 |

phonon displacements $\mathbf{u}^{\parallel}$ and phason displacements $\mathbf{u}^{\perp}$ at long wavelength when it is expanded in terms of the Taylor series to the second order. Since the elastic energy is a scalar quantity, each individual term in it must be invariant under all of the point group operations of the structure. In order to construct these quadratic invariants, we can invoke the group representation theory. As an example, we consider the point group $12mm$ ($C_{12v}$) which has nine irreducible representations (see Tab. 1). Two generators are the twelvefold rotation $\alpha$ and the mirror operation $\beta$, which can be represented by

$$\Gamma(\alpha) = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ -1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix},$$

$$\Gamma(\beta) = \begin{bmatrix} 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}. \tag{1}$$

The matrix representation $\Gamma$ reduces to

$$\Gamma = \Gamma_5 + \Gamma_1 + \Gamma_9. \tag{2}$$

It follows that $\mathbf{u}^{\parallel}$ transforms under $\Gamma_5 + \Gamma_1$ and $\mathbf{u}^{\perp}$ transforms under $\Gamma_9$. Following the same process as described in references [16–18], we obtain five quadratic invariants

$$\begin{aligned} &(E_{11}+E_{22})^2, \quad E_{33}^2, \quad (E_{11}+E_{22})E_{33}, \\ &(E_{11}-E_{22})^2 + (2E_{12})^2, \quad E_{13}^2 + E_{23}^2 \end{aligned} \tag{3}$$

and five independent elastic constants

$$C_{11}, C_{12}, C_{13}, C_{33}, C_{44}, C_{66} = \frac{1}{2}(C_{11} - C_{12}) \tag{4}$$

associated with the phonon field. For the phason field six components of $\partial_j u_i^{\perp}$ transform under

$$(\Gamma_5 + \Gamma_1) \times \Gamma_9 = \Gamma_3 + \Gamma_4 + \Gamma_8 + \Gamma_9. \tag{5}$$

The components $\partial_1 u_1^{\perp} - \partial_2 u_2^{\perp}$ and $\partial_1 u_2^{\perp} + \partial_2 u_1^{\perp}$ transform under $\Gamma_3$ and $\Gamma_4$ respectively, from which it follows that there are two quadratic invariants:

$$\left(\partial_1 u_1^{\perp} - \partial_2 u_2^{\perp}\right)^2, \left(\partial_1 u_2^{\perp} + \partial_2 u_1^{\perp}\right)^2. \tag{6}$$

The pairs ($\partial_1 u_1^{\perp} + \partial_2 u_2^{\perp}$, $\partial_1 u_2^{\perp} - \partial_2 u_1^{\perp}$) and ($\partial_3 u_1^{\perp}$, $\partial_3 u_2^{\perp}$) span the 2D irreducible representations $\Gamma_8$ and $\Gamma_9$ respectively. Thus, we can obtain two quadratic invariants:

$$\left(\partial_1 u_1^{\perp} + \partial_2 u_2^{\perp}\right)^2 + \left(\partial_1 u_2^{\perp} - \partial_2 u_1^{\perp}\right)^2, \left(\partial_3 u_1^{\perp}\right)^2 + \left(\partial_3 u_2^{\perp}\right)^2. \tag{7}$$

From (6) and (7), it follows that associated with the phason field there are four quadratic invariants and four independent elastic constants. Nonvanishing elastic constants are

$$\begin{aligned} &K_{1111} = K_{2222} = K_1, K_{1122} = K_{2211} = K_2, \\ &K_{1221} = K_{2112} = K_3, K_{1313} = K_{2323} = K_4, \\ &K_{1212} = K_{2121} = K_1 + K_2 + K_3. \end{aligned} \tag{8}$$

It should be noted that since no common term occurs in (5) and the reduction equation for phonon field, there are no invariants coupling $\mathbf{u}^{\parallel}$ and $\mathbf{u}^{\perp}$ and hence no phonon-phason coupling elastic constants. Therefore, it can be seen that there are nine quadratic invariants and hence nine independent elastic constants for $12mm$. Among them five elastic constants are associated with the phonon field and the rest with the phason field.

In the same way we can find all invariants and independent elastic constants for 12 ($C_{12}$) symmetry. There are ten quadratic invariants and hence ten independent elastic constants. Among them nine elastic constants are the same as those for $12mm$, another nonvanishing phason elastic constant is

$$\begin{aligned} K_{1112} &= K_{1211} = K_{1121} = K_{2111} \\ &= -K_{2212} = -K_{1222} = -K_{2221} = -K_{2122} = K_5. \end{aligned} \tag{9}$$

Dodecagonal system has seven point groups divided into two Laue classes which we term Laue classes 17 and 18 respectively. Laue class 17 includes 12, $\overline{12}$, $12/m$ while Laue class 18 includes $12mm$, 1222, $\overline{12}m2$, $12/mmm$. Elastic properties possess an inherent centrosymmetry. Therefore, all point groups belonging to the same Laue class possess the same elastic properties.

## 3 Formulae for diffuse scattering from dodecagonal quasicrystals

### 3.1 General formulae for diffuse scattering from quasicrystals

Here we derive general formulae for diffuse scattering from quasicrystals by a method similar to that often used for ordinary crystals [29]. Following the same process as described in reference [16] the observed scattering intensity is the average of the diffracted intensities for all the possible configurations,

$$I\left(\mathbf{q}^{\|}\right)=\frac{1}{(2\pi)^{2d-6}}\sum_{\mathbf{R}_1,\mathbf{R}_2}\iint \mathrm{e}^{\mathrm{i}\mathbf{k}_2\cdot\mathbf{R}_2-\mathrm{i}\mathbf{k}_1\cdot\mathbf{R}_1} fF(\mathbf{k}_1)F^*(\mathbf{k}_2)\times\delta^{\|}\left(\mathbf{q}^{\|}-\mathbf{k}_1^{\|}\right)\delta^{\|}\left(\mathbf{q}^{\|}-\mathbf{k}_2^{\|}\right)\mathrm{d}^d k_1 \mathrm{d}^d k_2, \quad (10)$$

where

$$F(\mathbf{k})=\int\rho_{\mathrm{c}}(\mathbf{x})\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}}\mathrm{d}^d x \quad (11)$$

is the structure factor of unit hypercell with $\rho_{\mathrm{c}}(\mathbf{x})$ denoting density distribution in a unit hypercell and where $f$ denotes the average

$$f=\left\langle \mathrm{e}^{\mathrm{i}\mathbf{k}_2\cdot\mathbf{u}\left(\mathbf{R}_2^{\|}\right)-\mathrm{i}\mathbf{k}_1\cdot\mathbf{u}\left(\mathbf{R}_1^{\|}\right)}\right\rangle. \quad (12)$$

Compared to the method given by Jaric and Nelson [7], the difference lies in the calculation of the average. As an approximation, we have

$$f\approx \mathrm{e}^{-\frac{1}{2}\left\langle\left[\mathbf{k}_1\cdot\mathbf{u}\left(\mathbf{R}_1^{\|}\right)-\mathbf{k}_2\cdot\mathbf{u}\left(\mathbf{R}_2^{\|}\right)\right]^2\right\rangle} \quad (13)$$

which can be written as an expansion

$$f(\mathbf{R}_1,\mathbf{R}_2,\mathbf{k}_1,\mathbf{k}_2)=\exp\left[-\frac{1}{2}\left\langle\left[\mathbf{k}_1\cdot\mathbf{u}\left(\mathbf{R}_1^{\|}\right)\right]^2\right\rangle-\frac{1}{2}\left\langle\left[\mathbf{k}_2\cdot\mathbf{u}\left(\mathbf{R}_2^{\|}\right)\right]^2\right\rangle\right]\times\left(1+\left\langle\left[\mathbf{k}_1\cdot\mathbf{u}\left(\mathbf{R}_1^{\|}\right)\right]\left[\mathbf{k}_2\cdot\mathbf{u}\left(\mathbf{R}_2^{\|}\right)\right]\right\rangle+\cdots\right) \quad (14)$$

and can be seen to depend only on the difference $\mathbf{R}_1-\mathbf{R}_2=\mathbf{R}$. Making this substitution and after writing $\left\langle\left[\mathbf{k}_1\cdot\mathbf{u}\left(\mathbf{R}_1^{\|}\right)\right]\left[\mathbf{k}_2\cdot\mathbf{u}\left(\mathbf{R}_2^{\|}\right)\right]\right\rangle$ in terms of Fourier transform $\mathbf{u}\left(\mathbf{p}^{\|}\right)$, we obtain

$$\left\langle\left[\mathbf{k}_1\cdot\mathbf{u}\left(\mathbf{R}_1^{\|}\right)\right]\left[\mathbf{k}_2\cdot\mathbf{u}\left(\mathbf{R}_2^{\|}\right)\right]\right\rangle=\frac{(2\pi)^3}{V}\times\int\left[\mathbf{k}_1\cdot\mathbf{u}\left(\mathbf{p}^{\|}\right)\right]\times\left[\mathbf{k}_2\cdot\mathbf{u}^*\left(\mathbf{p}^{\|}\right)\right]\exp(\mathrm{i}\mathbf{p}^{\|}\cdot\mathbf{R}^{\|})\mathrm{d}^3 p^{\|}, \quad (15)$$

where $V$ is the volume of the studied quasicrystal.

The modes associated with the phason field $\mathbf{u}^{\perp}$ are diffusive rather than propagating due to the friction that opposes relative motion of the incommensurate mass-density waves. It has been pointed out in reference [11] that if the friction coefficient coupling the incommensurate waves is small, there may exist a regime of wave numbers where the $\mathbf{u}^{\perp}$ mode are effectively propagating modes as has been observed in experiment [30]. According to the generalized elasticity theory of quasicrystals [23], in this case the equations of motion are

$$\begin{aligned}C_{ijkl}\frac{\partial^2 u_k^{\|}\left(\mathbf{x}^{\|}\right)}{\partial x_j\partial x_l}+R_{ijkl}\frac{\partial^2 u_k^{\perp}\left(\mathbf{x}^{\|}\right)}{\partial x_j\partial x_l}&=\rho\frac{\partial^2 u_i^{\|}\left(\mathbf{x}^{\|}\right)}{\partial^2 t},\\ R_{klij}\frac{\partial^2 u_k^{\|}\left(\mathbf{x}^{\|}\right)}{\partial x_j\partial x_l}+K_{ijkl}\frac{\partial^2 u_k^{\perp}\left(\mathbf{x}^{\|}\right)}{\partial x_j\partial x_l}&=\rho\frac{\partial^2 u_i^{\perp}\left(\mathbf{x}^{\|}\right)}{\partial^2 t},\end{aligned} \quad (16)$$

with $\rho$ being the average mass-density of the quasicrystal.

In order to find the explicit expression for $\mathbf{u}\left(\mathbf{p}^{\|}\right)$, we can employ (16) and the energy equipartition theorem. Following the derivation given in reference [17] we can easily obtain

$$\left[\mathbf{k}_1\cdot\mathbf{u}\left(\mathbf{p}^{\|}\right)\right]\left[\mathbf{k}_2\cdot\mathbf{u}^*\left(\mathbf{p}^{\|}\right)\right]=\frac{Vk_{\mathrm{B}}T}{(2\pi)^6}\mathbf{k}_1\cdot\mathbf{A}^{-1}\left(\mathbf{p}^{\|}\right)\cdot\mathbf{k}_2. \quad (17)$$

Therefore, (14) can be replaced by

$$f(\mathbf{R},\mathbf{k}_1,\mathbf{k}_2)=\mathrm{e}^{-W(\mathbf{k}_1)-W(\mathbf{k}_2)}\left(1+\frac{k_{\mathrm{B}}T}{(2\pi)^3}\times\int\mathbf{k}_1\cdot\mathbf{A}^{-1}\left(\mathbf{p}^{\|}\right)\cdot\mathbf{k}_2\exp\left(\mathrm{i}\mathbf{p}^{\|}\cdot\mathbf{R}^{\|}\right)\mathrm{d}^3 p^{\|}+\cdots\right), \quad (18)$$

where

$$W(\mathbf{k})=\frac{k_{\mathrm{B}}T}{2(2\pi)^3}\int\mathbf{k}\cdot\mathbf{A}^{-1}\left(\mathbf{p}^{\|}\right)\cdot\mathbf{k}\mathrm{d}^3 p^{\|} \quad (19)$$

and where $\mathbf{A}\left(\mathbf{p}^{\|}\right)$ is hydrodynamic matrix which is defined by

$$\begin{aligned}\left[\mathbf{A}^{\|,\|}\left(\mathbf{p}^{\|}\right)\right]_{ik}&=C_{ijkl}p_j^{\|}p_l^{\|},\\ \left[\mathbf{A}^{\perp,\perp}\left(\mathbf{p}^{\|}\right)\right]_{ik}&=K_{ijkl}p_j^{\|}p_l^{\|},\\ \left[\mathbf{A}^{\|,\perp}\left(\mathbf{p}^{\|}\right)\right]_{ik}&=\left[\mathbf{A}^{\perp,\|}\left(\mathbf{p}^{\|}\right)\right]_{ki}=R_{ijkl}p_j^{\|}p_l^{\|}.\end{aligned} \quad (20)$$

Then, following the derivation given by Jaric and Nelson [7], the scattering intensity can be evaluated and the result can be written as an expansion

$$I\left(\mathbf{q}^{\|}\right)=I_0\left(\mathbf{q}^{\|}\right)+I_1\left(\mathbf{q}^{\|}\right)+\cdots, \quad (21)$$

whose first two terms are the Bragg scattering

$$I_0\left(\mathbf{q}^{\|}\right)=\frac{(2\pi)^3 V}{v_{\mathrm{c}}^2}\sum_{\mathbf{Q}}\delta^{\|}\left(\mathbf{q}^{\|}-\mathbf{Q}^{\|}\right)\left|F(\mathbf{Q})\right|^2\mathrm{e}^{-2W(\mathbf{Q})}, \quad (22)$$

and the lowest-order diffuse scattering

$$I_1\left(\mathbf{q}^{\|}\right)=\frac{Vk_{\mathrm{B}}T}{v_{\mathrm{c}}^2}\sum_{\mathbf{Q}}\left(\mathbf{q}^{\|}\ \mathbf{Q}^{\perp}\right)\cdot\mathbf{A}^{-1}\left(\mathbf{q}^{\|}-\mathbf{Q}^{\|}\right)\times\begin{pmatrix}\mathbf{q}^{\|}\\ \mathbf{Q}^{\perp}\end{pmatrix}\left|F\left(\mathbf{q}^{\|},\mathbf{Q}^{\perp}\right)\right|^2\mathrm{e}^{-2W\left(\mathbf{q}^{\|},\mathbf{Q}^{\perp}\right)}, \quad (23)$$

$$\mathbf{A}^{\parallel,\parallel}\left(\mathbf{p}^{\parallel}\right)=\begin{bmatrix} C_{11}p_1^{\parallel 2}+C_{66}p_2^{\parallel 2}+C_{44}p_3^{\parallel 2} & (C_{11}-C_{66})p_1^{\parallel}p_2^{\parallel} & (C_{44}+C_{13})p_1^{\parallel}p_3^{\parallel} \\ (C_{11}-C_{66})p_1^{\parallel}p_2^{\parallel} & C_{66}p_1^{\parallel 2}+C_{11}p_2^{\parallel 2}+C_{44}p_3^{\parallel 2} & (C_{44}+C_{13})p_2^{\parallel}p_3^{\parallel} \\ (C_{44}+C_{13})p_1^{\parallel}p_3^{\parallel} & (C_{44}+C_{13})p_2^{\parallel}p_3^{\parallel} & C_{44}(p_1^{\parallel 2}+p_2^{\parallel 2})+C_{33}p_3^{\parallel 2} \end{bmatrix}, \tag{26}$$

$$\mathbf{A}^{\perp,\perp}\left(\mathbf{p}^{\parallel}\right)=\begin{bmatrix} K_1p_1^{\parallel 2}+(K_1+K_2+K_3)p_2^{\parallel 2}+K_4p_3^{\parallel 2}+2K_5p_1^{\parallel}p_2^{\parallel} & K_5(p_1^{\parallel 2}-p_2^{\parallel 2})+(K_2+K_3)p_1^{\parallel}p_2^{\parallel} \\ K_5(p_1^{\parallel 2}-p_2^{\parallel 2})+(K_2+K_3)p_1^{\parallel}p_2^{\parallel} & (K_1+K_2+K_3)p_1^{\parallel 2}+K_1p_2^{\parallel 2}+K_4p_3^{\parallel 2}-2K_5p_1^{\parallel}p_2^{\parallel} \end{bmatrix}. \tag{27}$$

$$\mathbf{A}^{\perp,\perp}\left(\mathbf{p}^{\parallel}\right)=\begin{bmatrix} K_1p_1^{\parallel 2}+(K_1+K_2+K_3)p_2^{\parallel 2}+K_4p_3^{\parallel 2} & (K_2+K_3)p_1^{\parallel}p_2^{\parallel} \\ (K_2+K_3)p_1^{\parallel}p_2^{\parallel} & (K_1+K_2+K_3)p_1^{\parallel 2}+K_1p_2^{\parallel 2}+K_4p_3^{\parallel 2} \end{bmatrix}. \tag{28}$$

where $\mathrm{e}^{-2W(\mathbf{q})}$ is the Debye-Waller factor.

Near a particular Bragg spot $\mathbf{Q}$ the scattering intensity can be written as

$$I\left(\mathbf{Q}^{\parallel}+\mathbf{p}^{\parallel}\right)\approx\frac{(2\pi)^3V}{v_{\mathrm{c}}^2}\left|F(\mathbf{Q})\right|^2\mathrm{e}^{-2W(\mathbf{Q})} \times\left[\delta^{\parallel}\left(\mathbf{p}^{\parallel}\right)+\frac{k_{\mathrm{B}}T}{(2\pi)^3}\mathbf{Q}\cdot\mathbf{A}^{-1}\left(\mathbf{p}^{\parallel}\right)\cdot\mathbf{Q}\right]. \tag{24}$$

The results obtained here coincide with those given by Jaric and Nelson [7] except some amendments for coefficients.

If the phasons drop out of thermal equilibrium at an elevated temperature $T_q$, then at a lower temperature $T$, phonons will equilibrate in the presence of a quenched phason displacement field. This situation has been examined [7,13,16] and it has been concluded [16] that $\mathbf{A}^{\parallel,\parallel}\left(\mathbf{p}^{\parallel}\right)$, $\mathbf{A}^{\parallel,\perp}\left(\mathbf{p}^{\parallel}\right)$ and $\mathbf{A}^{\perp,\parallel}\left(\mathbf{p}^{\parallel}\right)$ blocks are still given by equation (20) but $\mathbf{A}^{\perp,\perp}\left(\mathbf{p}^{\parallel}\right)$ block should be modified by

$$\mathbf{A}^{\perp,\perp}\left(\mathbf{p}^{\parallel}\right)=\frac{T}{T_q}\left\{\mathbf{A}_q^{\perp,\perp}\left(\mathbf{p}^{\parallel}\right)-\mathbf{A}_q^{\perp,\parallel}\left(\mathbf{p}^{\parallel}\right)\times\left[\mathbf{A}_q^{\parallel,\parallel}\left(\mathbf{p}^{\parallel}\right)\right]^{-1}\cdot\mathbf{A}_q^{\parallel,\perp}\left(\mathbf{p}^{\parallel}\right)\right\}+\mathbf{A}^{\perp,\parallel}\left(\mathbf{p}^{\parallel}\right)\cdot\left[\mathbf{A}^{\parallel,\parallel}\left(\mathbf{p}^{\parallel}\right)\right]^{-1}\cdot\mathbf{A}^{\parallel,\perp}\left(\mathbf{p}^{\parallel}\right), \tag{25}$$

where the subscript $q$ means that the values of the elastic constants at $T_q$ should be used. It should be emphasized that matrix $\mathbf{A}\left(\mathbf{p}^{\parallel}\right)$ is associated not only with phonon and phonon-phason coupling elastic constants $C_{ijkl}(T)$, $R_{ijkl}(T)$ at $T$, but also with all of the elastic constants $C_{ijkl}(T_q)$, $K_{ijkl}(T_q)$ and $R_{ijkl}(T_q)$ at $T_q$. Obviously, (25) will be reduced to that defined in (20) if $T=T_q$, which is physically reasonable. The result coincides with that given by Ishii [13].

### 3.2 Explicit expressions for a specific case of dodecagonal quasicrystals

It has been pointed out in Section 2 that all point groups belonging to the same Laue class possess the same elastic properties due to the inherent centrosymmetry of elastic properties. Therefore, matrix $\mathbf{A}\left(\mathbf{p}^{\parallel}\right)$ is identical for all point groups belonging to the same Laue class. From elastic properties of dodecagonal quasicrystals, explicit expressions of $\mathbf{A}^{\parallel,\parallel}\left(\mathbf{p}^{\parallel}\right)$, $\mathbf{A}^{\perp,\perp}\left(\mathbf{p}^{\parallel}\right)$ and $\mathbf{A}^{\parallel,\perp}\left(\mathbf{p}^{\parallel}\right)$ blocks for each Laue class of dodecagonal system can be easily obtained.

For Laue class 17, $\mathbf{A}^{\parallel,\parallel}\left(\mathbf{p}^{\parallel}\right)$ and $\mathbf{A}^{\perp,\perp}\left(\mathbf{p}^{\parallel}\right)$ blocks are given by

*see equations (26, 27) above.*

For Laue class 18, $\mathbf{A}^{\parallel,\parallel}\left(\mathbf{p}^{\parallel}\right)$ block takes the same form as (26). However, in this case elastic constant $K_5$ vanishes compared with Laue class 17. Consequently, $\mathbf{A}^{\perp,\perp}\left(\mathbf{p}^{\parallel}\right)$ block is

*see equation (28) above.*

It should be noted that $\mathbf{A}^{\parallel,\perp}\left(\mathbf{p}^{\parallel}\right)\equiv 0$ for both Laue classes 17 and 18 since there is no coupling between phonons and phasons in dodecagonal quasicrystals. Therefore, for quenched phasons, (25) should be replaced by

$$\mathbf{A}^{\perp,\perp}\left(\mathbf{p}^{\parallel}\right)=\frac{T}{T_q}\mathbf{A}_q^{\perp,\perp}\left(\mathbf{p}^{\parallel}\right). \tag{29}$$

It can be seen that matrix $\mathbf{A}\left(\mathbf{p}^{\parallel}\right)$ is associated only with phonon elastic constants $C_{ijkl}(T)$ at $T$ and phason elastic constants $K_{ijkl}(T_q)$ at $T_q$.

## 4 Contours of constant diffuse scattering intensity

It follows from (24) that

$$I_1\left(\mathbf{Q}^{\parallel}+\mathbf{p}^{\parallel}\right)=\frac{k_{\mathrm{B}}T}{(2\pi)^3}S\left(\mathbf{p}^{\parallel}\right)I_{\mathrm{Bragg}}(\mathbf{Q}^{\parallel}) \tag{30}$$

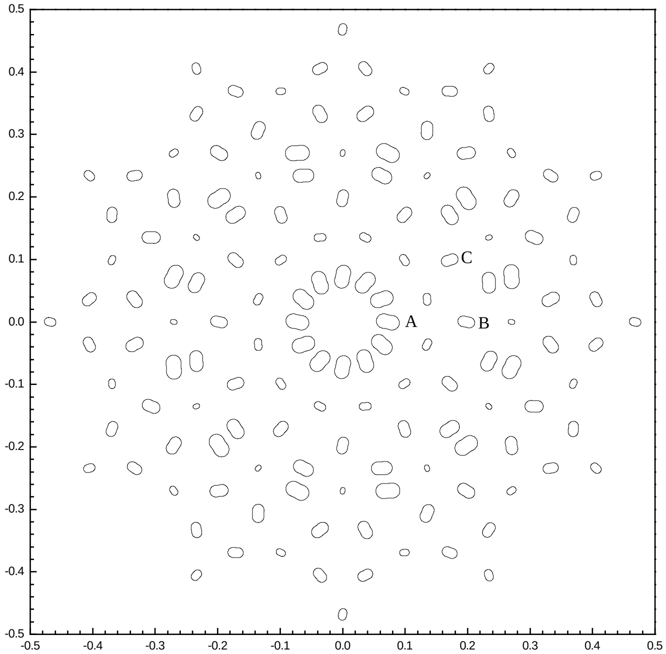


**Fig. 1.** Contours of constant diffuse scattering intensity in a plane perpendicular to the periodic axis with quenched phasons when $T = \frac{1}{3}T_q$ for the case of Laue class 17. Contours represent $S(\mathbf{p}^{\parallel}) = 16\,000$. Elastic constants are taken as $C_{11}(T) = 1.0$, $C_{13}(T) = -0.1$, $C_{33}(T) = 0.4$, $C_{44}(T) = 0.2$, $C_{66}(T) = 0.8$, $K_1(T_q) = 0.6$, $K_2(T_q) = 0.5$, $K_3(T_q) = 0.4$, $K_4(T_q) = 0.7$, and $K_5(T_q) = 0.2$. The indices of spots A, B and C are (2 −2 0 1 0), (−1 2 0 −1 0) and (1 −1 1 0 0) respectively.

where

$$I_{\text{Bragg}}(\mathbf{Q}^{\parallel}) = \frac{(2\pi)^3 V}{v_c^2} \left|F(\mathbf{Q})\right|^2 \mathrm{e}^{-2W(\mathbf{Q})} \tag{31}$$

is the integrated intensity of Bragg scattering around Bragg peak $\mathbf{Q}^{\parallel}$ and where $S\left(\mathbf{p}^{\parallel}\right)$ is defined by

$$S\left(\mathbf{p}^{\parallel}\right) = \mathbf{Q} \cdot \mathbf{A}^{-1}\left(\mathbf{p}^{\parallel}\right) \cdot \mathbf{Q}. \tag{32}$$

Using (32) and explicit expression of $\mathbf{A}\left(\mathbf{p}^{\parallel}\right)$ for dodecagonal quasicrystals, we simulated contours of constant diffuse scattering intensity for dodecagonal quasicrystals. In calculation, we fix $C_{11} = 1.0$ and use the ratios of elastic constants relative to $C_{11}$ because peak shapes are determined by the relative values of elastic constants but not the absolute values of them. Lattice constants are taken as $a = 3.7$ Å, $c = 5.2$ Å. It should be noted that isointensity contours represent ratios of diffuse scattering to Bragg scattering but not intensity of corresponding Bragg peaks.

Point groups $12/m$, $12/mmm$ represent symmetries of Laue classes 17 and 18 respectively. Figure 1 represents a plane perpendicular to the periodic direction with quenched phason displacements for the case of Laue class 17. It is assumed that phason quench temperature $T_q = 3T$. The diffuse scattering patterns in this plane show twelvefold rotation symmetry which is consistent with point group $12/m$.

Figures 2–6 give the results for the case of Laue class 18 which we would like to discuss in detail. Figures 2a and 2b illustrate diffuse scattering patterns in the plane perpendicular to the periodic direction for quenched phasons corresponding to two sets of different ratios of elastic constants. It is still assumed that $T_q = 3T$. It is obvious that the contour shapes around the same Bragg spots are quite different in Figures 2a and 2b. Figure 2c represents the same plane provided that both phonons and phasons are thermalized at $T$. It was also assumed that the ratios of elastic constants are the same as those in Figure 2a. The value of $S\left(\mathbf{p}^{\parallel}\right)$ that the contours represent in Figure 2c is half of that in Figure 2a, which indicates that the diffuse scattering decreases accompanied by slight variation of contour shapes around the same Bragg spots due to the reduced contribution of phason disorder in comparison with Figure 2a. If the diffuse scattering patterns like those in Figures 2a-2c could be detected and measured precisely, one could use these patterns to extract information about elastic constants. Such experiments have been done on a single grain of Al-Pd-Mn icosahedral phase using elastic neutron scattering [14,15]. It follows from (26) and (28) that terms containing elastic constants $C_{13}$, $C_{33}$ and $K_4$ vanish in matrix $\mathbf{A}\left(\mathbf{p}^{\parallel}\right)$ if the diffuse scattering patterns are measured in the plane perpendicular to the periodic direction as Figures 2a–2c so that such patterns are insufficient to acquire all of the elastic constants. Figures 2d and 2e show patterns perpendicular, respectively, to twofold axes A2P which is along the direction of arbitrary basis vector in quasiperiodic plane or its equivalent direction, and A2D which is along a bisector between any of these basis vectors and its neighboring equivalent direction with the same conditions as for Figure 2a and they may be used to give information about the other elastic constants that can not be present in Figures 2a–2c.

The symmetries of diffuse scattering patterns shown in Figure 2 are consistent with point group $12/mmm$. There are two kinds of mirrors in Figures 2a–2c besides a twelvefold rotation axis A12 along the periodic direction. One mirror is perpendicular to A2P and the other perpendicular to A2D.

In Figures 3-5 we present comparisons of contours of constant diffuse scattering intensity around Bragg spots (1 0 −1 1 0) and (0 1 1 −1 0) which are collinear Bragg spots, namely, their reciprocal lattice vectors $\mathbf{Q}^{\parallel}$ are parallel, for quenched phasons when $T = \frac{1}{3}T_q$. Figure 3 shows stereoscopic contours while Figures 4a, 4b and 4c gives diffuse scattering line shapes in planes perpendicular, respectively, to A12, AQ which is along corresponding reciprocal lattice vector $\mathbf{Q}^{\parallel}$, and AV which is perpendicular to A12 and AQ directions. It can be seen that shapes of isointensity contours vary greatly even for collinear Bragg spots in comparison with those of ordinary crystals. The relation of $S(\mathbf{p}^{\parallel})$ to $1/\left|\mathbf{p}^{\parallel}\right|^2$ along A12, AQ and AV directions given in Figure 5 shows that diffuse scattering intensity is proportional to $1/\left|\mathbf{p}^{\parallel}\right|^2$ which holds for ordinary crystals. The slope in a given direction $\mathbf{p}^{\parallel}$ is associated with corresponding specific elastic constants,

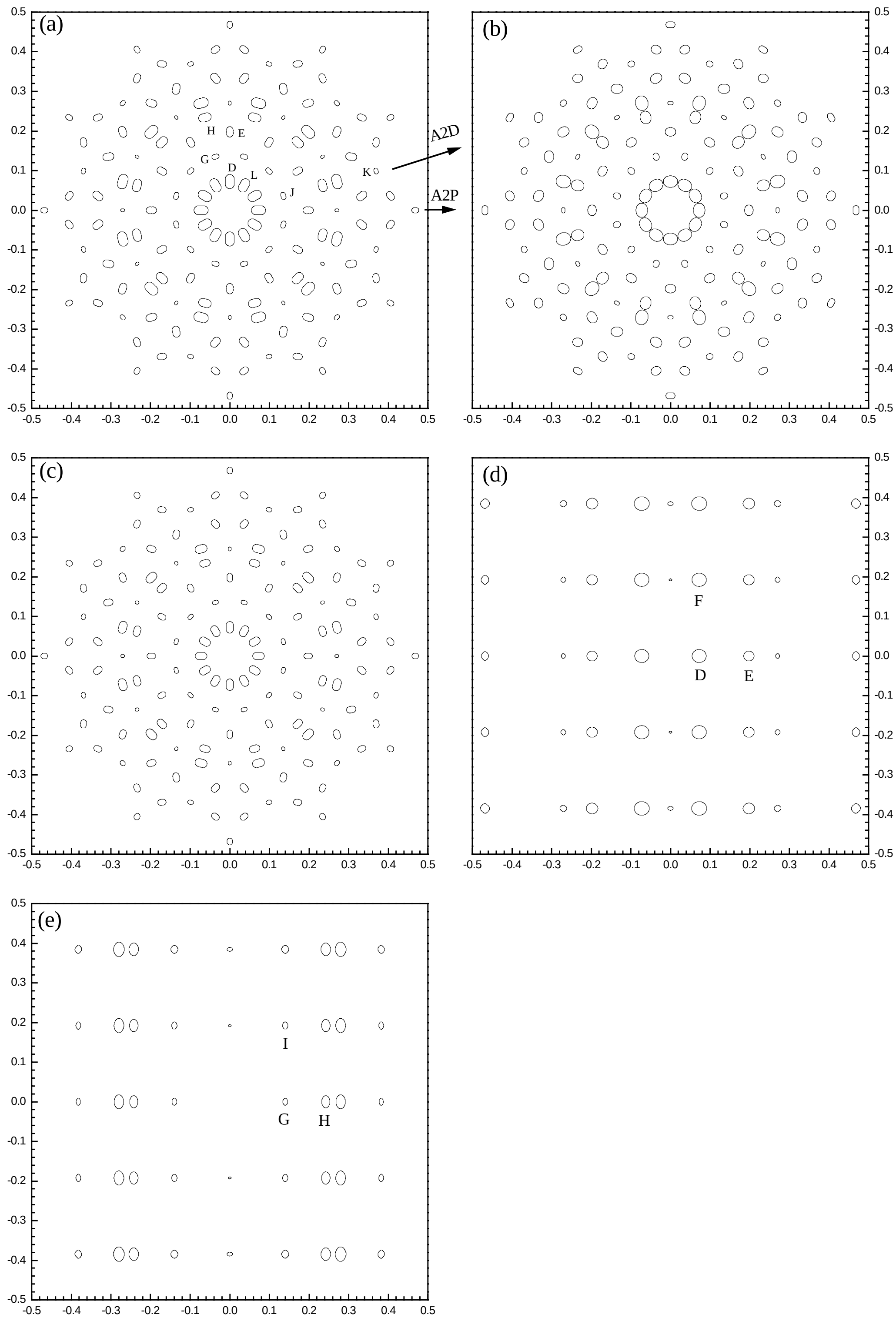


**Fig. 2.** Isointensity contours in planes for the case of Laue class 18. (a), (d), and (e) correspond, respectively, to planes perpendicular to A12, A2P, and A2D axes with quenched phasons when $T = \frac{1}{3}T_q$. Contours represent $S\left(\mathbf{p}^{\parallel}\right) = 16\,000$. Elastic constants are taken as $C_{11}(T) = 1.0$, $C_{13}(T) = -0.1$, $C_{33}(T) = 0.4$, $C_{44}(T) = 0.2$, $C_{66}(T) = 0.8$, $K_1(T_q) = 0.6$, $K_2(T_q) = 0.5$, $K_3(T_q) = 0.4$, and $K_4(T_q) = 0.7$. The indices of spots D, E, F in (d) are $(1\ 0\ {-2}\ 2\ 0)$, $({-1}\ 0\ 2\ {-1}\ 0)$, $(1\ 0\ {-2}\ 2\ 1)$ and those of spots G, H, I in (e) are $({-1}\ 1\ 0\ 0\ 0)$, $(1\ {-2}\ 1\ 1\ 0)$, $({-1}\ 1\ 0\ 0\ 1)$ respectively. (b) Similar to (a) except that elastic constants are taken as $C_{11}(T) = 1.0$, $C_{13}(T) = 0.1$, $C_{33}(T) = 0.6$, $C_{44}(T) = 0.8$, $C_{66}(T) = 0.2$, $K_1(T_q) = 0.9$, $K_2(T_q) = -0.1$, $K_3(T_q) = -0.2$, and $K_4(T_q) = 0.4$. (c) The same as (a) except that both phonons and phasons are assumed thermalized and contours represent $S(\mathbf{p}^{\parallel}) = 8\,000$.

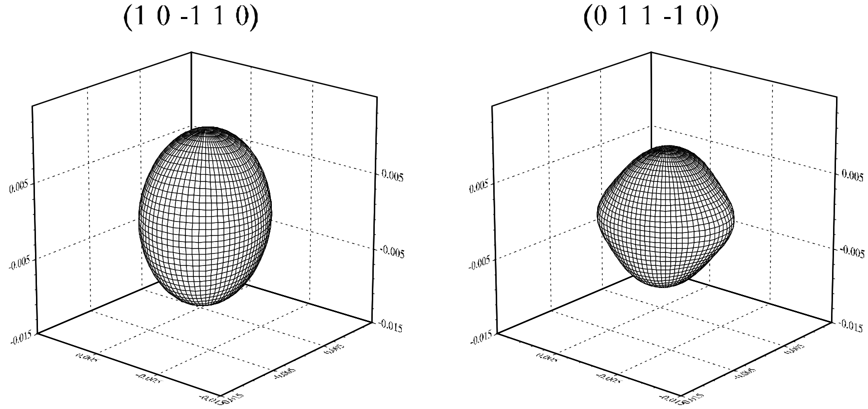


**Fig. 3.** Stereoscopic isointensity contours around Bragg spots J (1 0 −1 1 0) and K (0 1 1 −1 0) with quenched phasons when $T = \frac{1}{3}T_q$ for the case of Laue class 18. Elastic constants are taken as those in Figure 2b. Contours represent $S(\mathbf{p}^{\parallel}) = 16\,000$.

$$\begin{bmatrix}\mathbf{e}_1^*\\ \mathbf{e}_2^*\\ \mathbf{e}_3^*\\ \mathbf{e}_4^*\\ \mathbf{e}_5^*\end{bmatrix} = a^* \begin{bmatrix} \cos\left(\frac{0\pi}{6}\right) & \sin\left(\frac{0\pi}{6}\right) & 0 & \cos\left(\frac{0\pi}{6}\right) & \sin\left(\frac{0\pi}{6}\right)\\ \cos\left(\frac{1\pi}{6}\right) & \sin\left(\frac{1\pi}{6}\right) & 0 & \cos\left(\frac{5\pi}{6}\right) & \sin\left(\frac{5\pi}{6}\right)\\ \cos\left(\frac{2\pi}{6}\right) & \sin\left(\frac{2\pi}{6}\right) & 0 & \cos\left(\frac{10\pi}{6}\right) & \sin\left(\frac{10\pi}{6}\right)\\ \cos\left(\frac{3\pi}{6}\right) & \sin\left(\frac{3\pi}{6}\right) & 0 & \cos\left(\frac{15\pi}{6}\right) & \sin\left(\frac{15\pi}{6}\right)\\ 0 & 0 & \frac{c^*}{a^*} & 0 & 0 \end{bmatrix} \begin{bmatrix}\mathbf{E}_1^{\parallel}\\ \mathbf{E}_2^{\parallel}\\ \mathbf{E}_3^{\parallel}\\ \mathbf{E}_1^{\perp}\\ \mathbf{E}_2^{\perp}\end{bmatrix} = a^* \begin{bmatrix} 1 & 0 & 0 & 1 & 0\\ \frac{\sqrt{3}}{2} & \frac{1}{2} & 0 & -\frac{\sqrt{3}}{2} & \frac{1}{2}\\ \frac{1}{2} & \frac{\sqrt{3}}{2} & 0 & \frac{1}{2} & -\frac{\sqrt{3}}{2}\\ 0 & 1 & 0 & 0 & 1\\ 0 & 0 & \frac{c^*}{a^*} & 0 & 0 \end{bmatrix} \begin{bmatrix}\mathbf{E}_1^{\parallel}\\ \mathbf{E}_2^{\parallel}\\ \mathbf{E}_3^{\parallel}\\ \mathbf{E}_1^{\perp}\\ \mathbf{E}_2^{\perp}\end{bmatrix}, \quad (33)$$

*i.e.*, slope along A12 direction is only related to $C_{33}$, $C_{44}$ and $K_4$.

Figure 6 presents comparisons of stereoscopic contours of constant diffuse scattering intensity around Bragg spots (2 1 −2 −2 1) and (0 −1 2 −1 0) among which the latter is indicated in Figure 2a, for quenched phasons when $T = \frac{1}{3}T_q$. In calculation, we consider three sets of elastic constants. Only phonon elastic constants in Figure 6b and phason elastic constants in Figure 6c are changed with respect to those in Figure 6a. It is evident that the shape of isointensity contour around reflection (0 −1 2 −1 0) which has large $\mathbf{Q}^{\perp}$ component varies greatly in Figure 6c but slightly in Figure 6b in comparison with that in Figure 6a while the very reverse results can be found for reflection (2 1 −2 −2 1) which has large $\mathbf{Q}^{\parallel}$ component. The fact that peak shapes of Bragg spots with large $\mathbf{Q}^{\perp}$ component are dominated by phason elastic constants can be accounted for by special phason degrees of freedom in quasicrystals which also give rise to the variation of peak shapes among collinear Bragg spots as shown in Figures 3 and 4.

## 5 Conclusion

Explicit formulae for diffuse scattering from dodecagonal quasicrystals have been derived in terms of the elastic constants. Isointensity contours of diffuse scattering were calculated to examine the effect of phonon and phason disorders on diffuse scattering from dodecagonal quasicrystals. The symmetries of diffuse scattering patterns are consistent with corresponding point groups. Unlike ordinary crystals, shapes of isointensity contours are much more complicated and varies even among the collinear Bragg spots due to the additional phason degrees of freedom. Quantitative examination of diffuse scattering patterns may yield numerical values of the elastic constants.

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## Appendix

In this appendix, we give the coordinate systems for dodecagonal quasicrystals used in this paper. The structure of dodecagonal quasicrystals is conveniently described in 5D hyperspace $E = (E^{\parallel}, E^{\perp})$ that may be decomposed into two orthogonal subspaces: $E^{\parallel}$, the 3D physical or parallel space with orthogonal unit basis vectors $\mathbf{E}_1^{\parallel}$, $\mathbf{E}_2^{\parallel}$, $\mathbf{E}_3^{\parallel}$, and $E^{\perp}$, 2D complementary or perpendicular space with orthogonal unit basis vectors $\mathbf{E}_1^{\perp}$ , $\mathbf{E}_2^{\perp}$. Every spot in the diffraction pattern of dodecagonal quasicrystals may be indexed using a combination of five reciprocal basis vectors $\mathbf{e}_i^*, i = 1, 2, \ldots, 5$ which can be written as

*see equation (33) above*

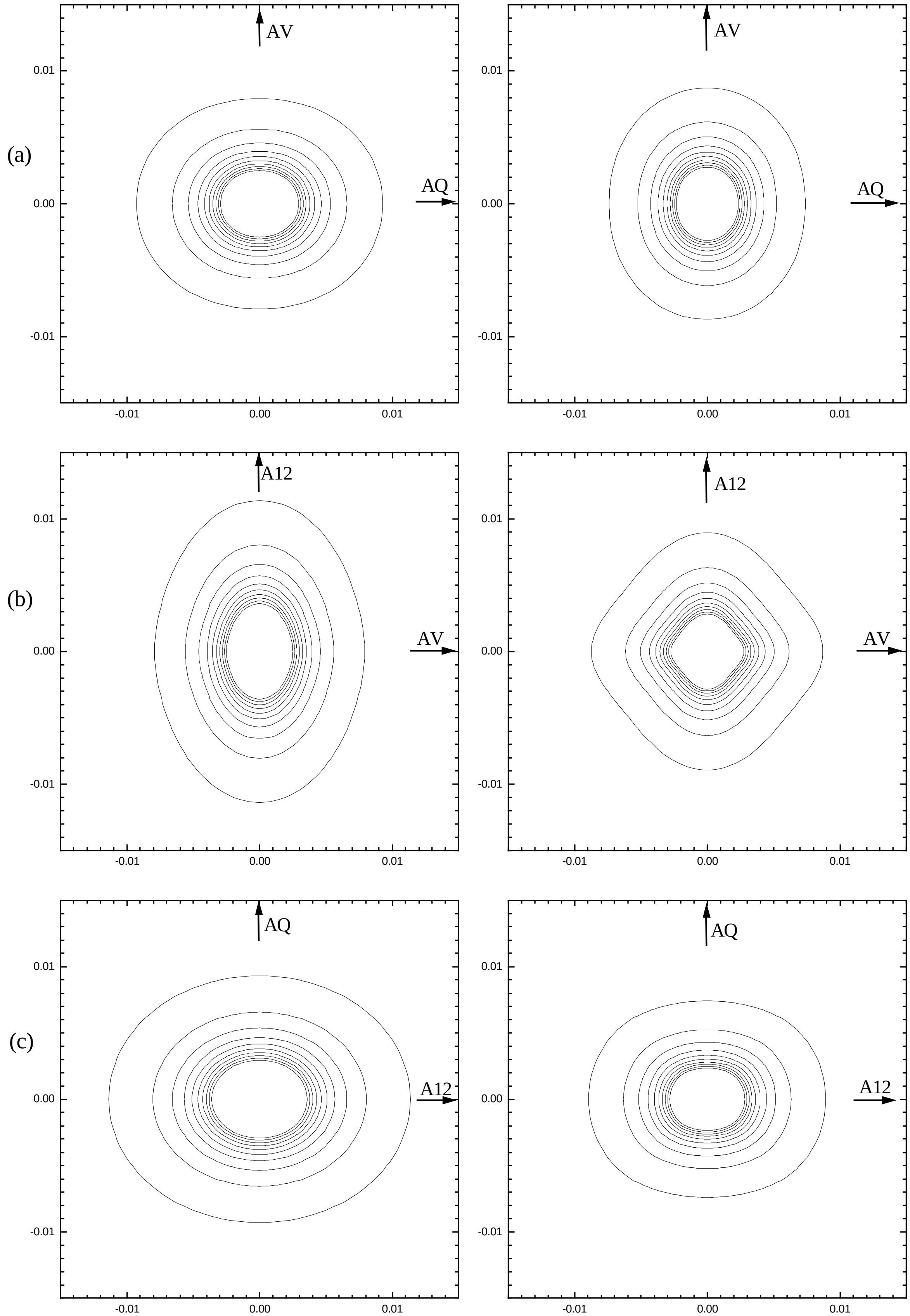


**Fig. 4.** Diffuse scattering line shapes in planes perpendicular, respectively, to (a) A12, (b) AQ, and (c) AV directions with contours representing $S(\mathbf{p}^{\parallel}) = 16\,000n$ $(n = 1, 2, \ldots, 10)$. The other parameters are taken as those in Figure 3.

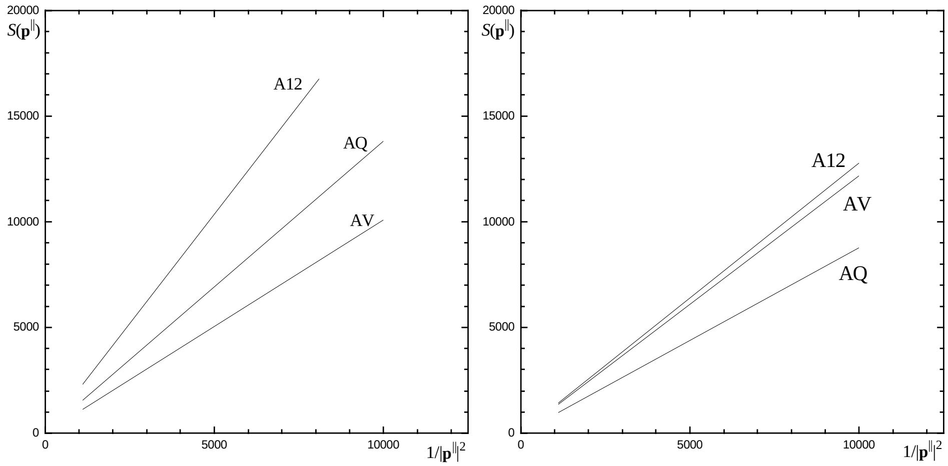


**Fig. 5.** Relation of $S\left(\mathbf{p}^{\parallel}\right)$ to $1/\left|\mathbf{p}^{\parallel}\right|^{2}$ along A12, AQ and AV directions. The other parameters are taken as those in Figure 3.

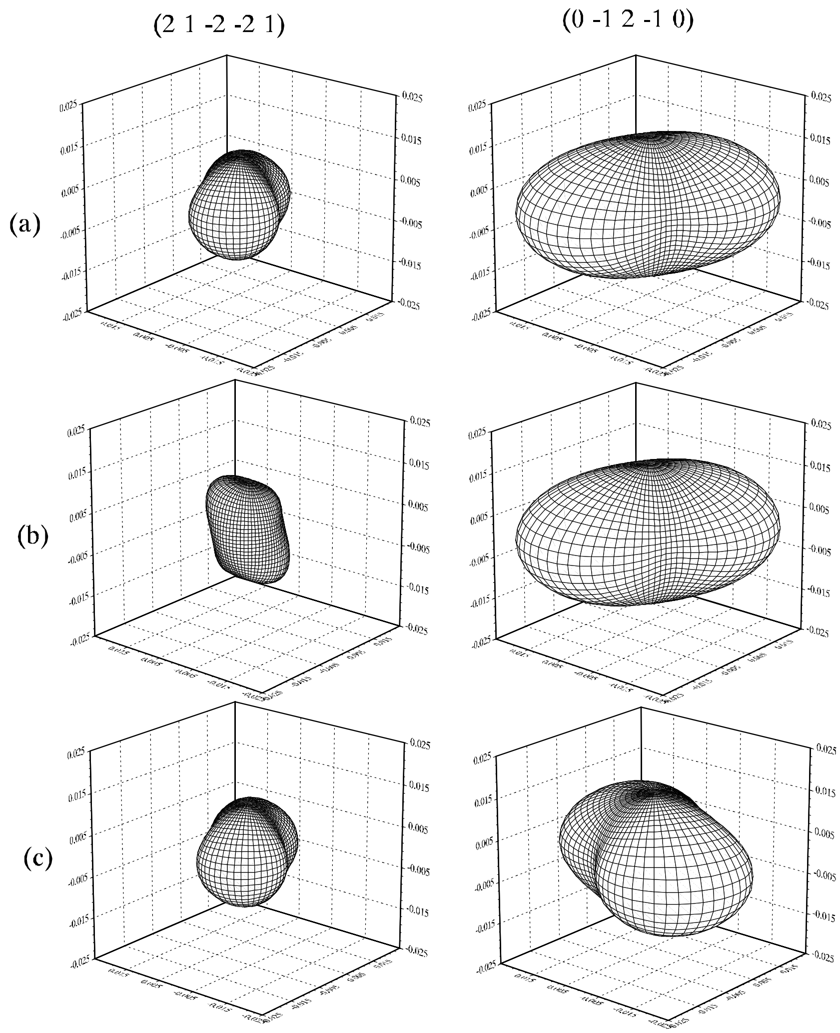


**Fig. 6.** Comparisons of stereoscopic isointensity contours around Bragg spots (2 1 −2 −2 1) and L (0 −1 2 −1 0) with quenched phasons when $T = \frac{1}{3}T_q$ for the case of Laue class 18. Contours represent $S(\mathbf{p}^{\parallel}) = 16\,000$. Elastic constants are taken as follows: (a) $C_{11}(T) = 1.0$, $C_{13}(T) = -0.3$, $C_{33}(T) = 0.3$, $C_{44}(T) = 0.5$, $C_{66}(T) = 0.2$, $K_1(T_q) = 0.9$, $K_2(T_q) = -0.3$, $K_3(T_q) = -0.4$, and $K_4(T_q) = 0.7$; (b) $C_{11}(T) = 1.0$, $C_{13}(T) = 0.2$, $C_{33}(T) = 0.5$, $C_{44}(T) = 0.5$, $C_{66}(T) = 0.7$ and the same phason elastic constants as those in (a); (c) the same phonon elastic constants as those in (a) and $K_1(T_q) = 0.2$, $K_2(T_q) = 0.3$, $K_3(T_q) = 0.4$, $K_4(T_q) = 0.8$.

where $a^*$ and $c^*$ are the reciprocal lattice constants. Consequently, the direct basis vectors $\mathbf{e}_i, i = 1, 2, \ldots, 5$ reciprocal to $\mathbf{e}_i^*, i = 1, 2, \ldots, 5$ are given by

$$\begin{bmatrix} \mathbf{e}_1 \\ \mathbf{e}_2 \\ \mathbf{e}_3 \\ \mathbf{e}_4 \\ \mathbf{e}_5 \end{bmatrix} = \frac{a}{\sqrt{3}} \begin{bmatrix} \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 & \frac{\sqrt{3}}{2} & \frac{1}{2} \\ 1 & 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 & -1 \\ -\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 & \frac{1}{2} & \frac{\sqrt{3}}{2} \\ 0 & 0 & \frac{\sqrt{3}c}{a} & 0 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{E}_1^{\parallel} \\ \mathbf{E}_2^{\parallel} \\ \mathbf{E}_3^{\parallel} \\ \mathbf{E}_1^{\perp} \\ \mathbf{E}_2^{\perp} \end{bmatrix}, \qquad (34)$$

where $a, c$ are the lattice constants and $a = 1/a^*$, $c = 1/c^*$.

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